

Quantum Transport Enhancement by Time-Reversal Symmetry Breaking

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Quantum mechanics still provides new unexpected effects when considering the transport of energy and information. Models of continuous time quantum walks, which implicitly use time-reversal symmetric Hamiltonians, have been intensely used to investigate the effectiveness of transport. Here we show how breaking time-reversal symmetry in this model can enable directional control, enhancement, and suppression of quantum transport. Examples ranging from exciton transport to complex networks are presented. This opens new prospects for more efficient methods to transport energy and information.

Understanding quantum transport is key to developing more robust communication networks, more effective energy transmission, and improved information processing devices. Continuous time quantum walks have become a standard model to study and understand quantum transport phenomena [1, 2, 3, 4, 5]. Time-reversal symmetry (TRS) characterizes all quantum walk models to date. This symmetry implies that the site-to-site transfer probability at time $t = T$ is the same as at time $t = -T$, thereby prohibiting directional biasing. Here we introduce and study continuous time “chiral” quantum walks whose dynamics break TRS. Our findings show that the breaking of TRS offers the possibility of directional biasing and allows one to suppress or enhance transport relative to the standard quantum walk. One reason this effect was overlooked could be that time-reversal asymmetry cannot affect the site-to-site transport in some simple cases, such as linear chains and trees. This is proven in the supplementary online material (SOM) Section 2. Prior efforts have focused on controlling and directing quantum transport using either *in situ* tunable Hamiltonians [6, 7] or tailoring specific initial states [8]. In contrast to known approaches, we consider states initially prepared in the standard *site-basis* and time-independent Hamiltonians that induce time-asymmetric evolutions.

To demonstrate the effect of TRS breaking, we chose four examples which illustrate the main ideas of directionality, suppression and enhancement of transport. The first example is a unitary quantum switch, where the direction of quantum transport is controlled by a time-reversal asymmetry parameter. The second example examines transport in a linear chain of triangles, showing a 633% transport speedup for the chiral quantum walk. Next, we demonstrate complete suppression of chiral quantum walks on loops with an even number of sites. We then consider a system widely studied in the exciton transport literature: the Fenna-Matthew-Olsen complex (FMO). Although this naturally occurring system is highly efficient, we find that the introduction of chiral terms allows for an enhancement of transport speed by 7.68%. Finally, to investigate the robustness of TRS breaking effects on transport, we consider randomly gen-

erated small-world networks. By appending time-reversal asymmetric terms to only the edges of the graph connected to the final site, we could increase the speed of the site-to-site transport significantly, up to 130%.

In the standard literature on continuous time quantum walks [1, 2, 3, 4, 5], the time-independent walk Hamiltonian is defined by a real weighted adjacency matrix J of an underlying undirected graph,

$$H_{QW} = \sum_{n,m}^{sites} J_{nm}(|n\rangle\langle m| + |m\rangle\langle n|). \quad (1)$$

The condition that the hopping weights J_{nm} are real numbers implies that the induced transitions between two sites are symmetric under time inversion. We can break this symmetry while maintaining the hermicity of the operator by appending a complex phase to an edge: $J_{nm} \rightarrow J_{nm}e^{i\theta_{nm}}$ resulting in a continuous time *chiral quantum walk* (CQW) governed by

$$H_{CQW} = \sum_{n,m} J_{nm}e^{i\theta_{nm}}|n\rangle\langle m| + J_{nm}e^{-i\theta_{nm}}|m\rangle\langle n|. \quad (2)$$

When acting on the single exciton subspace the Hamiltonian given in Eq. (2) can be expressed in terms of the spin-half Pauli matrices:

$$H_{CQW} = \sum_{n,m} J_{nm} \cos(\theta_{nm})(\sigma_n^x \sigma_m^x + \sigma_n^y \sigma_m^y) + \sum_{n,m} J_{nm} \sin(\theta_{nm})(\sigma_n^x \sigma_m^y - \sigma_n^y \sigma_m^x) \quad (3)$$

which arises in a variety of physical systems. In the CQW framework, we investigate coherent quantum dynamics and incoherent dynamics within the Markov approximation. Both types of evolution are included in the Lindblad equation [9, 10, 11, 12]:

$$\frac{d}{dt}\rho(t) = \mathcal{L}\{\rho\} = -i[H_{CQW}, \rho] + \sum_k L_k \rho L_k^\dagger - \frac{1}{2} \left(L_k^\dagger L_k \rho + \rho L_k^\dagger L_k \right) \quad (4)$$

where $\rho(t)$ is the density operator describing the state of the system at time t and L_k are Lindblad operators inducing stochastic jumps between quantum states. For example, using the usual terminology of Markovian processes, we call site t a trap if it is coupled to site s by the Lindblad

jump operators, $L_k = |t\rangle\langle s|$. The site-to-site transfer probability, $P_{n \rightarrow m}(t) = \langle m | \rho(t) | m \rangle$, gives the occupancy probability of site m at time t with initial condition $\rho(0) = |n\rangle\langle n|$. To quantify the transport properties of quantum walks, we use the *half-arrival time*, $\tau_{1/2}$, as the earliest time when the occupancy probability of the target site is one half. We will also make use of the transport speed, $\nu_{1/2}$, defined as the reciprocal of $\tau_{1/2}$.

We now introduce a quantum switch which enables directed transport and could, in principle, be used to create a logic gate and offer future implementations of transport devices to store and process energy and information. Fig. 1 presents an example of this switch. The value of a phase ($e^{i\theta}$) appended to a single control edge across the junction allows selective biasing of transport through the switch. The maximal biasing occurs at $|\theta| = \pi/2$, and the sign determines the direction. The first maxima of $P_{S \rightarrow E}(t)$ (transfer probability from site S to E) in the unitary dynamics without traps can be enhanced by 134% or suppressed to 91% with respect to the non-chiral case. When considering traps in the Lindbladian evolution, the optimal transport efficiency is 81.4% in the preferred direction. The switch violates TRS as $P_{S \rightarrow E}(-t) \neq P_{S \rightarrow E}(t)$. By using $P_{S \rightarrow E}(-t) = P_{E \rightarrow S}(t)$ and the symmetry of the configuration $P_{E \rightarrow S}(t) = P_{S \rightarrow F}(t)$, we conclude that transport is biased towards the opposite pole when running backwards in time, see Fig 1. Note that the behavior of the switch is largely independent of the length of the connecting wires.

We will now utilize the directional biasing of the triangle to give an example of a speedup of chiral walks. Using the composition of eight triangular switches as depicted in Fig. 2A, by simultaneously varying all phases along the red control edges to the same value, we examine the effect of time-reversal asymmetry on transport. We find that the occupation probability as a function of θ is symmetric about $\pm\pi/2$ with the negative value corresponding to maximal enhancement and the positive value to maximal suppression. Unlike the occupation probability maxima in the switch, here the first apexes are separated in time. When we include trapping,

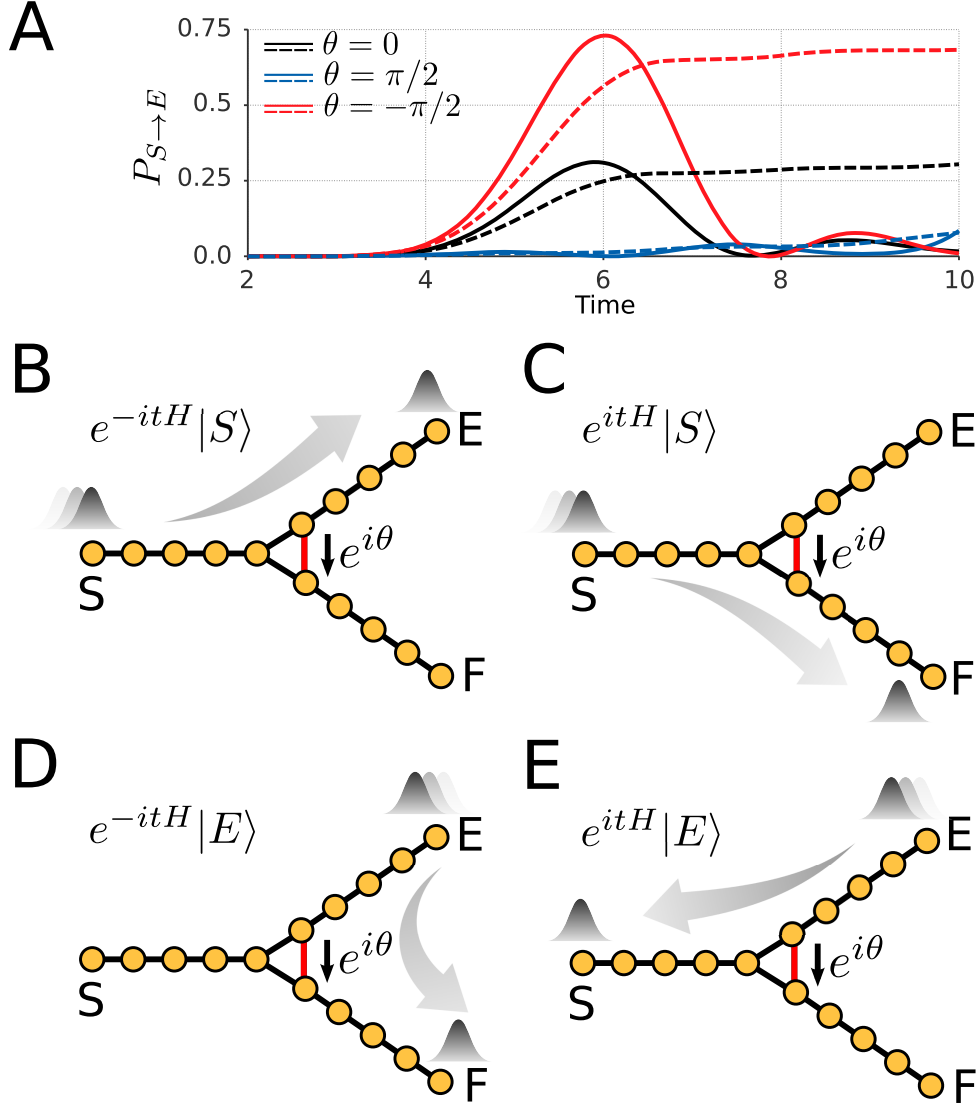


Figure 1: The quantum switch. (A) Directional biasing: enhanced transport in the preferred direction. The plot shows the occupancy probability $P_{S \rightarrow E}$ of site E with the particle initially starting from site S with and without sink (dashed and solid lines, respectively). (C) This evolution is time-reversal asymmetric as replacing t with $-t$ results in the particle moving from site S towards site F . (D) When starting at site E , the particle evolves towards site F . (E) By replacing t with $-t$ a particle initially at site E evolves towards the initial configuration (B). To recover time-reversal symmetric transition probabilities in the evolution (B), requires that one also performs the antiunitary operation [13] on the Hamiltonian mapping θ to $-\theta$. This has the same effect as reflecting the configuration (C) horizontally across the page while leaving the site labels intact.

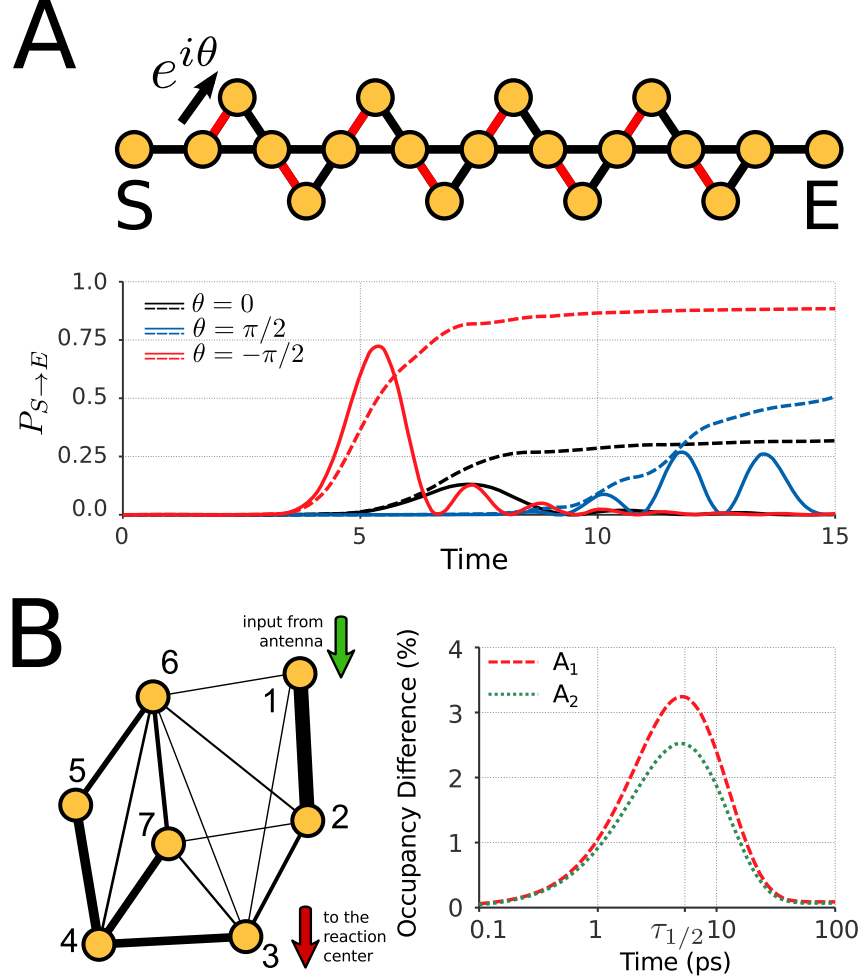


Figure 2: **(A)** Triangle chain and **(B)** the FMO complex. **(A)** The phase $e^{i\theta}$ is applied to the red edges simultaneously in the triangle chain. The plot illustrates the occupancy probability at the end site E as a function of time for different values of the phase θ with and without trapping (dashed and solid lines, respectively). **(B)** shows the occupancy difference with respect to the time reversal symmetric Hamiltonian of the FMO complex. We use an optimization procedure to enhance the transport. While holding the magnitude of the couplings constant, we optimize two sets of phases, A_1 and A_2 , which correspond to seven and three edges with an enhancement at $\tau_{1/2}$ of 3.25% and 2.25%, respectively.

the half-arrival time is reduced from the non-chiral value $\tau_{1/2} = 38.1$ to 5.2 which represents a 633% enhancement. To conclude this section we focus on suppression of transport by chiral quantum walks. A good example is the polygon with an even number of sites. In this case complete suppression can be achieved by appending a phase of π to one of the links in the cycle; thereby rendering it impossible for the quantum walker to move to the diametrically opposite site. The proof that this site-to-site transfer probability is zero for all time can be found in SOM S1.

In natural and synthetic excitonic networks such as photosynthetic complexes and solar cells, we are faced with non-unitary quantum evolution due to dissipative and decoherent interaction with the environment. Studies have shown that dissipative quantum evolution surpasses both classical and purely quantum transport (for interesting recent examples see [12, 14]). A widely studied process of such dissipative exciton transport is the one occurring in the Fenna-Matthews-Olsen complex (FMO), which connects the photosynthetic antenna to a reaction center in green sulfur bacteria [15, 16]. Due to the low light exposure of these bacteria, there is evolutionary pressure to optimize exciton transport. Therefore, the site energies and site-to-site couplings in the system are optimized, yielding a highly efficient transport. However, the natural exciton transport occurs via time-reversal symmetric interactions, and we ask whether TRS breaking interactions may further enhance the efficiency of the process. We consider the real Hamiltonian modeling transport on the FMO and allow for TRS breaking by introducing complex phases and find that the transport speed can be further increased. We study the seven site model of the FMO using an open system description that includes the thermal bath, trapping at the reaction center, and recombination of the exciton [15]. By performing a standard optimization procedure (as outlined in the SOM S3) that varies the phase on a subset of seven edges, we found a combination of phases where the transport speed, $\nu_{1/2}$, is enhanced by 7.68%. In Fig. 2B, the enhancement of the time dependent occupation probability is shown for the chiral

quantum walk. We note that optimization over only three edges already changes the transport speed by 5.92%, see SOM S3.

One may also ask if optimization procedures limited to small subsets of edges will generally lead to improved transport in larger and possibly randomly generated networks. We found a positive answer when testing the site-to-site transport between oppositely aligned nodes in the Watts-Strogatz model [17]. This family of small-world networks continuously connects a class of regular cyclic graphs to that of completely random networks (Erdős-Rényi models[18]) by changing the value of the rewiring probability.

We numerically investigated graphs with 32 nodes, average degree 4 and range over rewiring probability p considering 200 different graph realizations for each value of p . An example with $p = 0.2$ is depicted in Fig. 3A. Here the occupancy of a sink connected to site E is compared between the chiral walk and its achiral counterpart. The particle begins at site S and we perform the optimization of the phases only on edges connected to site E . In the case of the chiral quantum walk, the sink reaches half-occupancy in 54.8% less time on average. When the occupancy of the sink of the standard quantum walk reaches 0.5 at time $T = 175.17$, the sink occupancy of the chiral walk is already 33.5% higher on average.

In all the examples studied, we found that transport is affected by the topology of the network. A key explanation is the following. If two Hamiltonians are related by on-site unitary transformations mapping $|n\rangle$ to $e^{i\alpha_n}|n\rangle$, then the site-to-site transition probabilities will be identical. This fact provides a tool to reduce the effective space of phase parameters for controlling transport, see SOM S1. For instance, the site-to-site transfer probability is insensitive to phases in tree graphs. For bipartite graphs the phases can have an effect, however, the dynamics still remains time-reversal symmetric.

A further consequence is that the sums of phases along a chosen orientation of a loop are the unique invariants under on-site unitary transformations. In a wide range of cases and par-

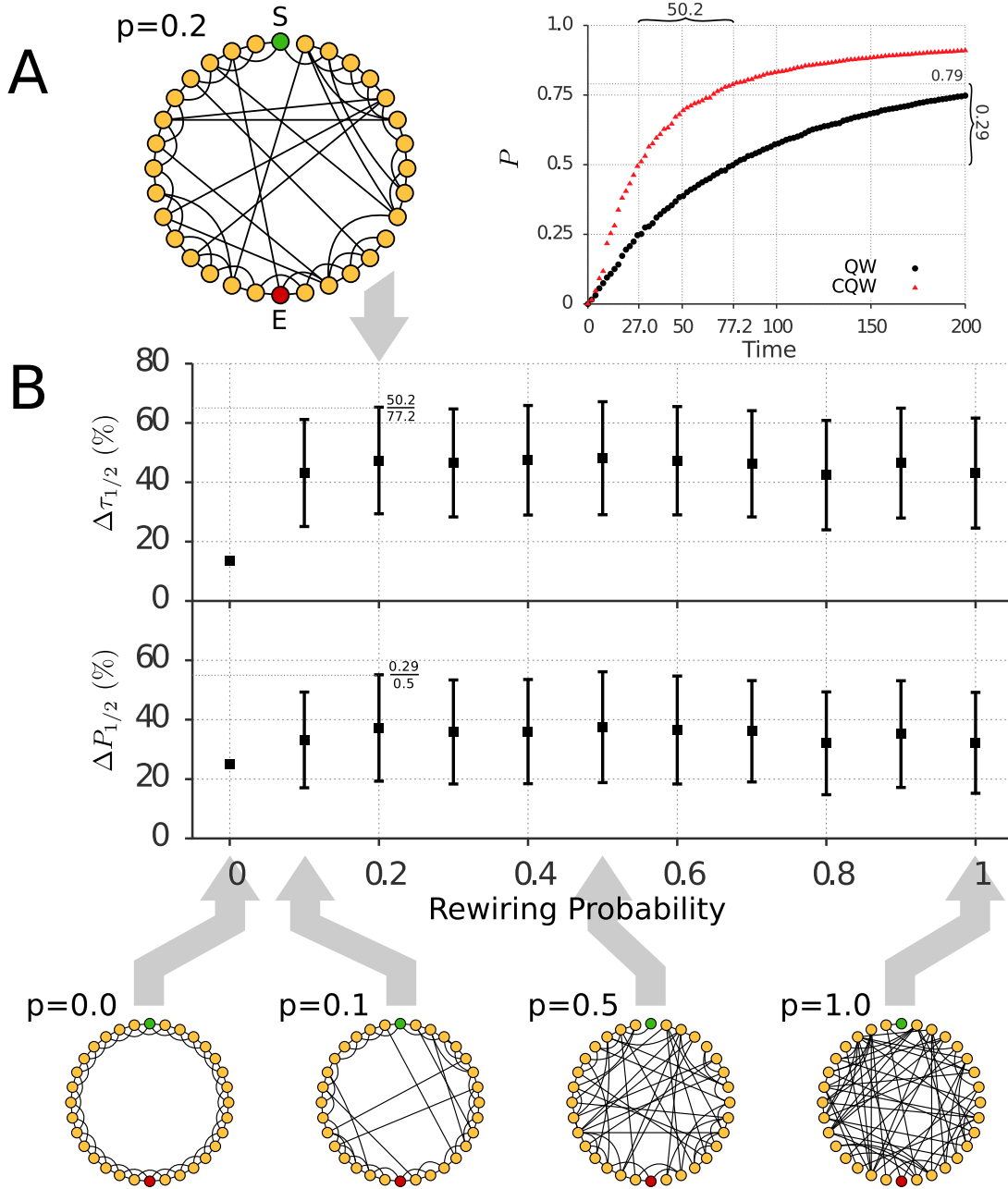


Figure 3: Transport enhancement of the chiral quantum walk is robust across randomly generated Watts-Strogatz networks. An example of this small-world network, with rewiring probability $p = 0.2$, is depicted in (A). The transfer probability P from site S to the sink connected to site E is plotted in a realization of the network. (B) shows the average enhancement of half arrival time ($\Delta\tau_{1/2}$) for different values of p .

ticularly in all examples we considered, we found strong evidence of the robustness the effect has on transport. For instance, the examples in Fig. 3B shows that in the Watts-Strogatz model, the transport enhancement due to the time reversal asymmetry of the Hamiltonian is insensitive to changes of the rewiring probability p and the clustering coefficient measuring the density of triangles in the graph. Finally, additional calculations show that scale free networks such as the Barabási-Albert model [19], show a similar transport enhancement, indicating robustness also with respect to the degree distribution.

This study pioneers the exploration of a new degree of freedom that allows for a significant improvement of control in the engineering of quantum transport. The fact that we were able to optimize and control transport by adjusting the phase on only a few edges inside a complex network and that the effect was relevant in a host of examples adds optimism to the robustness of this approach. Experimental demonstrations of the effects we predict are within reach of existing hardware, as outlined in SOM Section S2.

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References and Notes

- [1] E. Farhi and S. Gutmann. Quantum computation and decision trees. *Phys. Rev. A*, 58:915–928, 1998.
- [2] A. M. Childs, R. Cleve, E. Deotto, E. Farhi, S. Gutmann, and D. A. Spielman. Exponential algorithmic speedup by quantum walk. *Proc. 35th Annual ACM STOC. ACM, NY*, pages

59–68, 2003.

- [3] O. Mülken and A. Blumen. Continuous-time quantum walks: Models for coherent transport on complex networks. *Phys. Rep.*, 502:37–87, 2011.
- [4] J. Kempe. Quantum random walks: an introductory overview. *Contemp. Phys.*, 44:307–327, 2003.
- [5] V. Kendon. Decoherence in quantum walks - a review. *Math. Struct. in Comp. Sci.*, 17:1169–1220, 2006.
- [6] C. Godsil and S. Severini. Control by quantum dynamics on graphs. *Phys. Rev. A*, 81:052316, 2010.
- [7] D. Burgarth, D. D’Alessandro, L. Hogben, S. Severini, and M. Young. Zero forcing, linear and quantum controllability for systems evolving on networks. *arXiv*:, 1111.1475v1, 2011.
- [8] A. Eisfeld. Phase directed excitonic transport and its limitations due to environmental influence. *J. Chem. Phys.*, 379:33, 2011.
- [9] A. Kossakowski. On quantum statistical mechanics of non-Hamiltonian systems. *Rep. Math. Phys.*, 3:247, 1972.
- [10] G. Lindblad. On the generators of quantum dynamical semigroups. *Commun. Math. Phys.*, 48:119, 1975.
- [11] H.-P. Breuer and F. Petruccione. *The theory of open quantum systems*. Oxford University Press, New York 2002.

- [12] J. D. Whitfield, C. A. Rodriguez-Rosario, and A. Aspuru-Guzik. Quantum stochastic walks: A generalization of classical random walks and quantum walks. *Phys. Rev. A*, 81:022323, 2010.
- [13] E. P. Wigner. *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra*. New York: Academic Press, 1959. Translation by J. J. Griffin of 1931, *Gruppentheorie und ihre Anwendungen auf die Quantenmechanik der Atomspektren*, Vieweg Verlag, Braunschweig.
- [14] I. Sinayskiy, A. Marais, F. Petruccione, and A. Ekert. Decoherence-assisted transport in a dimer system. *Phys. Rev. Lett.*, 108:020602, Jan 2012.
- [15] M. Mohseni, P. Rebentrost, S. Lloyd, and A. Aspuru-Guzik. Environment-assisted quantum walks in photosynthetic energy transfer. *J. Chem. Phys.*, 129(17):174106, 2008.
- [16] A. Ishizaki and G. R. Fleming. Quantum coherence in photosynthetic light harvesting. *Annu. Rev. Cond. Mat. Phys.*, 3(1):333–361, 2012.
- [17] D. J. Watts and S. H. Strogatz. Collective dynamics of ‘small-world’ networks. *Nature*, 393(6684):409–410, 1998.
- [18] P. Erdős and A. Rényi. On the Evolution of Random Graphs. In *Publication of the Mathematical Institute of the Hungarian Academy of Sciences*, pages 17–61, 1960.
- [19] A.-L. Barabási and R. Albert. Emergence of scaling in random networks. *Science*, 286(5439):509–512, 1999.
- [20] F. Zähringer, G. Kirchmair, R. Gerritsma, E. Solano, R. Blatt, and C. F. Roos. Realization of a quantum walk with one and two trapped ions. *Phys. Rev. Lett.*, 104:100503, Mar 2010.

- [21] B. P. Lanyon, C. Hempel, D. Nigg, M. Müller, R. Gerritsma, F. Zähringer, P. Schindler, J. T. Barreiro, M. Rambach, G. Kirchmair, M. Hennrich, P. Zoller, R. Blatt, and C. F. Roos. Universal digital quantum simulation with trapped ions. *Science*, 334(6052):57–61, 2011.
- [22] K. Kim, M. S. Chang, S. Korenblit, R. Islam, E. E. Edwards, J. K. Freericks, G. D. Lin, L. M. Duan, and C. Monroe. Quantum simulation of frustrated Ising spins with trapped ions. *Nature*, 465(7298):590–593, 06 2010.
- [23] K. Kim, S. Korenblit, R. Islam, E. E. Edwards, M.-S. Chang, C. Noh, H. Carmichael, G.-D. Lin, L.-M. Duan, C. C. Joseph Wang, J. K. Freericks, and C. Monroe. Quantum simulation of the transverse ising model with trapped ions. *New J. Phys.*, 13(10):105003, 2011.
- [24] G. Kirchmair, J. Benhelm, F. Zähringer, R. Gerritsma, C. F. Roos, and R. Blatt. Deterministic entanglement of ions in thermal states of motion. *New Journal of Physics*, 11(2):023002, 2009.
- [25] J. Adolphs and T. Renger. How proteins trigger excitation energy transfer in the FMO complex of green sulfur bacteria. *Biophys. J.*, 91(8):2778–2797, 2006.

Supplementary Material

S1 Basic definitions and properties of chiral quantum walks

S1.1 Site-to-site transfer probability

The Markovian open-system dynamics of a continuous time chiral quantum walk is given by the Kossakowski-Lindblad equation [9, 10, 11, 12]

$$\mathcal{L}\{\rho\} = -i[H_{CQW}, \rho] + \sum_{(n,m)} c_{mn} \left(L_{nm}\rho L_{nm}^\dagger - \frac{1}{2}L_{nm}^\dagger L_{nm}\rho - \frac{1}{2}\rho L_{nm}^\dagger L_{nm} \right), \quad (\text{S1})$$

where the chiral Hamiltonian H_{CQW} is defined in Eq. (2), and the Lindblad operators are given as $L_{mn} = |m\rangle\langle n|$ with $c_{nm} \geq 0$. Transport from vertex $|S\rangle$ to vertex $|E\rangle$ during such dynamics is characterized by the site-to-site transfer probability (STP). In the unitary case ($c_{nm} = 0$) it is given by

$$P_{S \rightarrow E}(t) = \text{Tr}(e^{-iH_{CQW}t} \rho_S e^{iH_{CQW}t} \rho_E) \quad (\text{S2})$$

with $\rho_S = |S\rangle\langle S|$ and $\rho_E = |E\rangle\langle E|$, while for the general Markovian case it is

$$P_{S \rightarrow E}(t) = \text{Tr}(e^{\mathcal{L}t} \{\rho_S\} \rho_E). \quad (\text{S3})$$

S1.2 Time-reversal symmetry of the unitary achiral dynamics

In the setting of quantum walks, the time-reversal operator T acts as complex conjugation (with respect to the vertex basis) [13]:

$$T \sum_{v \in V} \alpha_v |v\rangle = \sum_{v \in V} \alpha_v^* |v\rangle.$$

The antiunitarity of T and $T^2 = 1$ implies that $T^\dagger = T$. The time-reversal of a Hamiltonian H is given as $THT^\dagger (= THT)$. The $H \mapsto THT$ action is represented in parameter space by the replacement $\theta_{mn} \mapsto -\theta_{mn}$ in Eq. (2). Thus exactly the achiral quantum walks are left invariant

by this action. The STP's of H ($P_{S \rightarrow E}(t)$) and that of $H' = THT$ ($P'_{S \rightarrow E}(t)$) are related in the following way:

$$P'_{S \rightarrow E}(t) = P_{S \rightarrow E}(-t) \text{ and } P'_{S \rightarrow E}(t) = P_{E \rightarrow S}(t),$$

which can be verified using $T\rho_v T = \rho_v$ and the cyclicity of the trace as follows:

$$\begin{aligned} P'_{S \rightarrow E}(t) &= \text{Tr}(e^{-i(THT)t} \rho_S e^{i(THT)t} \rho_E) = \text{Tr}(T e^{iHt} T \rho_S T e^{-iHt} T \rho_E) \\ &= \text{Tr}(e^{iHt} T \rho_S T e^{-iHt} T \rho_E T) = \text{Tr}(e^{iHt} \rho_S e^{-iHt} \rho_E) = P_{S \rightarrow E}(-t), \\ P_{S \rightarrow E}(-t) &= \text{Tr}(e^{iHt} \rho_S e^{-iHt} \rho_E) = \text{Tr}(e^{-iHt} \rho_E e^{iHt} \rho_S) = P_{E \rightarrow S}(t). \end{aligned}$$

A crucial consequence of the above is that in the case of achiral quantum walks, the transition probabilities are the same at time t and $-t$, i.e. $P_{S \rightarrow E}(t) = P_{S \rightarrow E}(-t)$, and directional biasing is prohibited $P_{S \rightarrow E}(t) = P_{E \rightarrow S}(t)$. However, $H \neq THT^\dagger$ does not necessarily imply that transition rates are asymmetric in time. This is because THT^\dagger might be gauge-equivalent to H , as will be seen in the next section.

S1.3 Gauge transformations

A local change of basis, such as a diagonal unitary:

$$U_d |n\rangle = e^{i\alpha_n} |n\rangle, \quad (\text{S4})$$

leaves the STP invariant. To prove this, let us first note that any unitary basis-change U would induce a transformation on the Lindblad superoperator $\mathcal{L} \rightarrow \mathcal{L}'$ with

$$\mathcal{L}'\{\rho\} = U \mathcal{L}\{U^\dagger \rho U\} U^\dagger.$$

Using this and the invariance of localized states under diagonal unitaries ($U_d^\dagger \rho_v U_d = \rho_v$), we arrive at

$$\begin{aligned} P'_{S \rightarrow E}(t) &= \text{Tr}(e^{\mathcal{L}'t} \{\rho_S\} \rho_E) = \text{Tr}(U_d e^{\mathcal{L}t} \{U_d^\dagger \rho_S U_d\} U_d^\dagger \rho_E) \\ &= \text{Tr}(e^{\mathcal{L}t} \{\rho_S\} U_d^\dagger \rho_E U_d) = \text{Tr}(e^{\mathcal{L}t} \{\rho_S\} \rho_E) = P_{S \rightarrow E}(t), \end{aligned}$$

which proves the invariance of the STP under the gauge transformations defined by Eq. (S4).

Under these diagonal transformations, the parameters of the quantum walk Hamiltonian transform as

$$\theta_{mn} \mapsto \theta_{mn} + \alpha_m - \alpha_n, \quad (\text{S5})$$

as illustrated in Fig. S1. The incoherent part of the Lindblad equation (S1) does not change since the Lindblad operators transform as $L_{nm} \rightarrow e^{i(\alpha_m - \alpha_n)} L_{nm}$ and these phases cancel in Eq. (S1), since L_{nm} and L_{nm}^\dagger appear paired. Two important properties of the model now follow: (i) phases on tree graphs can be transformed out completely and (ii) the sum of phases along loops is invariant under gauge transformations.

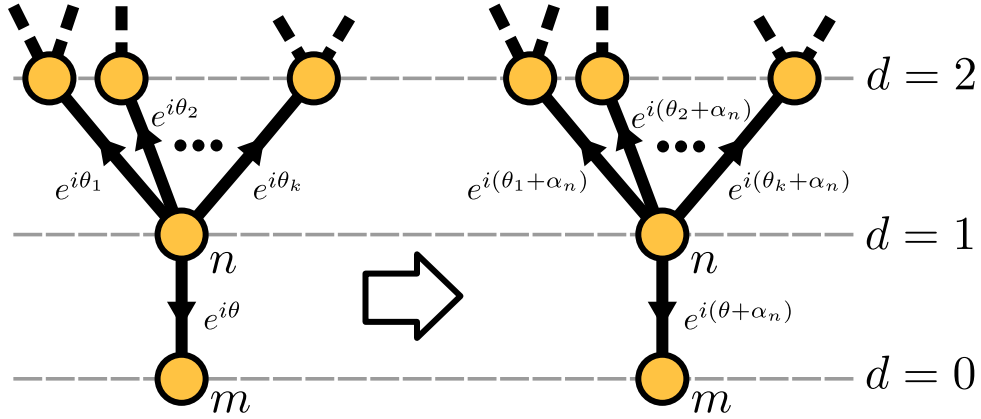


Fig. S1: Effect of the gauge transformation $|n\rangle \rightarrow e^{i\alpha_n}|n\rangle$ on vertex n . Phases on edges can be gauge-transformed without changing the transition amplitudes, as described in the text. Here we arrange the graph as a tree rooted at $d = 0$.

The first property is illustrated in Fig. S1. Let us take an arbitrary tree graph and pick a vertex m with only one neighbor. Redraw every other vertex on successive levels characterized by the distance d of the vertexes from the given vertex m . Note that the number of edges connecting two vertices, d , is by definition, unique in tree graphs. In such an arrangement only one edge emanates downwards from a given vertex on a line of $d > 0$ so Fig. S1 represents the general neighborhood of a vertex n having distance $d = 1$ from m . The indicated gauge

transformation with $\alpha_n = -\theta$ removes the phase from the bottom edge. Then, one iterates the procedure for all vertices at level $d = 2$ and consecutively for all levels. In this way, all phases are removed. For the second property, pick an orientation on a loop of N vertexes and compute $\theta := \sum_{i=1}^N \phi_{i,i+1}$, considering $\phi_{N,N+1} \equiv \phi_{N,1}$. A gauge transformation $|n\rangle \mapsto e^{i\alpha_n}|n\rangle$, according to Eq. (S5) leads to:

$$\phi_{n,n+1} \mapsto \phi_{n,n+1} + \alpha_n, \quad \phi_{n-1,n} \mapsto \phi_{n-1,n} - \alpha_n,$$

so the sum θ remains unaffected.

S1.4 Analytic examples for enhancement, suppression and direction

Using the example of the regular polygon (that has $J_{mn} \equiv 1$ for all edges) we will explain how enhancement, suppression and direction of transport can be influenced by the phases in chiral quantum walks. Typically we need to solve the eigenvalue problem of the Hamiltonian $H|\tilde{j}\rangle = E_j|\tilde{j}\rangle$ (the tilde denotes energy eigenstates) to compute

$$P_{S \rightarrow E}(t) = \left| \sum_j^N \langle E|\tilde{j}\rangle \langle \tilde{j}|S\rangle e^{-iE_j t} \right|^2$$

For a regular homogeneous polygon ($H = \sum_{n=1}^N e^{i\varphi}|n\rangle\langle n+1| + h.c.$ with cyclic boundary condition) the eigenvectors and eigenvalues are found from the Fourier Transform

$$|\tilde{k}\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{-\frac{2\pi i k n}{N}} |n\rangle, \quad E_k(\varphi) = 2 \cos\left(\frac{2\pi k}{N} - \varphi\right),$$

The STP from site S to E then reads

$$P_{S \rightarrow E}(t, \varphi) = \left| \frac{1}{N} \sum_{k=0}^{N-1} e^{-i\left(2t \cos\left(\frac{2\pi k}{N} - \varphi\right) + \frac{2\pi k(f-s)}{N}\right)} \right|^2 \quad (\text{S6})$$

We now list several features

- Direction and enhancement

In the case of time symmetric quantum walks, for the homogeneous polygon $P_{S \rightarrow E} = P_{S \rightarrow N-E+2S}$. This implies that if the number of edges is odd, the STP is at most $1/2$, since there is always a vertex different from E at which the probability is identical. The chiral case breaks this symmetry. In particular, for the regular triangle one can reach $P_{1 \rightarrow 2}(t) = 1$; one can find values of θ analytically by equating the phases of the three exponentials in the STP modulo 2π and solve the two linear equations for t and θ . Enhancement and direction is indicated in Fig. S2, where a triangle graph is shown with inhomogeneous coupling.

- Complete suppression of transport

Complete suppression of transport is possible in loops with an even number of sites. They belong to the set of *bipartite* graphs, whose vertices can be partitioned into two sets such that edges connect only members from different subsets. Directing transport in bipartite graphs is forbidden. This can be easily shown by noting that the gauge transformation $|n\rangle \mapsto -|n\rangle$ for all members of one subset has the effect of $H \mapsto -H$, which is precisely the time reversal transformation. Hence

$$P_{S \rightarrow E}(t) = P_{S \rightarrow E}(-t) = \text{Tr}(e^{iHt} \rho_S e^{-iHt} \rho_E) = \text{Tr}(e^{-iHt} \rho_E e^{iHt} \rho_S) = P_{E \rightarrow S}(t) .$$

Even chiral loops suppress transport as $\theta = \pi$ results in $p_{1 \rightarrow N/2+1}(t) = 0$ for all times t . This can again be shown by writing down the formula (S6) and separating it into two sums, one for k being even and the other for k odd. The simplest even polygon is the quadrilateral that can be used as a building block for the realization of transport suppressing topologies.

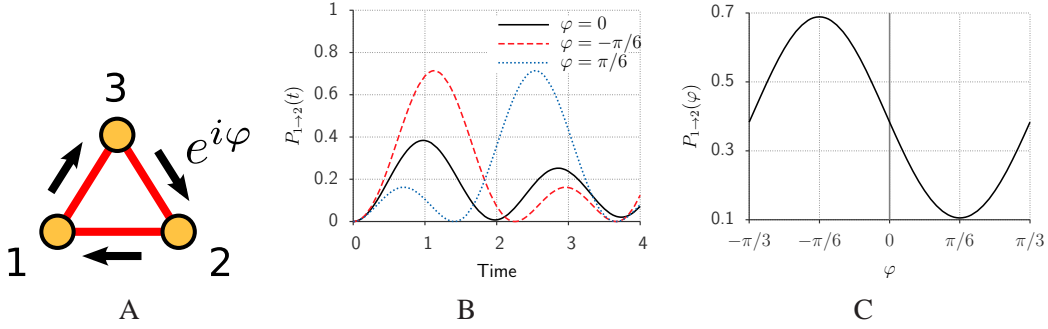


Fig. S2: (A) Triangle with inhomogeneous coupling and chiral phases. (B) Illustrates the quantity $P_{1 \rightarrow 2}(t)$ for the triangle graph with inhomogeneous coupling $J_{12} = 1$, $J_{23} = 1.3$, $J_{13} = 0.5$. Directing the phases of the chiral walker effects the transport, in particular, there is enhancement for $\theta = 3\varphi = \pi/2$ in both arrival time and maximal probability. (C) The probability varies as a function of the chiral angle at a given time near the first maximum.

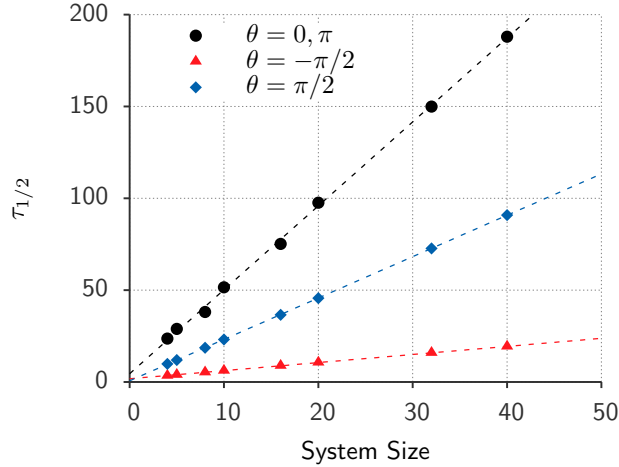


Fig. S3: Half arrival time scaling. Dependence of the half arrival time, $\tau_{1/2}$, on the length of the triangle chain shown in Figure 2A for different values of the phases. Both chiral ($\theta \neq 0$) and achiral ($\theta = 0$) cases exhibit linear scaling behaviour. The slope can be tuned by changing the value of the phase parameter.

S1.5 Robustness of chiral transport enhancement of the triangle chain

In the triangle chain discussed in the main text, the half arrival time $\tau_{1/2}$ depends linearly on the size of the system, see Figure S3. This fact is a characteristic of quantum walks in linear chains

and continues to hold for the chiral triangle chain.

S2 Experimental proposal

S2.1 Summary

In this section we outline a proposal to simulate chiral quantum walks in a system of ultra-cold trapped atomic ions. The proposal can be realized with currently available techniques and technology. Trapped ion systems have previously been used to investigate non-chiral quantum walks [20], where the motional state was used to encode the walk. In contrast, in our proposal both chiral and non-chiral walks are encoded into the electronic state of the ions. The walk dynamics is generated by ion-ion interactions mediated by joint vibrational modes of the ion string. These interactions can be driven by laser-induced optical dipole forces, for example, and can be implemented with high quality as shown in several recent works [21, 22]. In the text below we first introduce the 3-ion system that the experiment requires. Then we explain how to engineer the quantum walk Hamiltonians that we wish to investigate. Next, we calculate the chiral and non-chiral phenomena that can be generated by these Hamiltonians. Finally, we outline the experimental procedure and note some important experimental considerations.

S2.2 Implementation in trapped ions

We consider a string of three ions in a linear ion crystal, which can be achieved with standard linear-Paul traps. A long-lived electronic transition inside each ion encodes a two-level spin. The mapping could be that spin-down is represented by an ion in the ground state, while spin-up is represented by an ion in the excited state of this transition, for example. The 8 possible logical states of this system then become $|\downarrow, \downarrow, \downarrow\rangle, |\downarrow, \downarrow, \uparrow\rangle, |\downarrow, \uparrow, \downarrow\rangle, \dots, |\uparrow, \uparrow, \uparrow\rangle$. In our proposal a subset of these states represents the sites of the quantum walk, as will be described. The dynamics of any quantum walk between these states require the ability to turn on interac-

tions between the ionic spins. Effective ion-ion interactions can be achieved by off-resonantly coupling the electronic states in which the spin is encoded to one or more common vibrational modes of the string. Such a spin-dependant force can be implemented using a laser field with two symmetrically tuned frequencies at $\omega_s \pm \mu$ with $\mu \ll \omega_s$. If the symmetric detuning is sufficiently far from all motional sidebands so that the generation of phonons can be adiabatically eliminated [23], then a pure spin-spin interaction is generated of the form:

$$H(\phi) = \sum_{i < j} J_{ij} \sigma_{\phi}^i \sigma_{\phi}^j, \quad (\text{S7})$$

where

$$\begin{aligned} \sigma_{\phi}^i &= \cos \phi \sigma_x^i + \sin \phi \sigma_y^i \\ J_{ij} &= \frac{\Omega^2 \eta^2 \omega}{\Delta^2 - \omega^2} b_i b_j \end{aligned} \quad (\text{S8})$$

Here Ω describes the laser coupling strength to the electronic transition, η_i is the Lamb-Dicke parameter describing the coupling strength between the laser and the motional sideband for a single ion. An experimentally tunable phase ϕ is set by the phase difference of the two driving laser fields. Finally, b_i describes how strongly ion i couples to motional mode ω . The increasing difficulty of generating spin-spin interactions with more ions in a string is incorporated in b_i .

In this proposal we will simultaneously use two of the normal modes along the axis of the string, called the center-of-mass (COM) and breathing (Br) modes, to mediate spin-spin interactions. These modes are typically well-spaced in frequency and can therefore be individually addressed. The coupling vectors b_i for the axial COM and breathing are $1/\sqrt{3} \times [1, 1, 1]$ and $1/\sqrt{2} \times [1, 0, -1]$, respectively. Consequently, the contributions to the spin-spin interaction Hamiltonian of these modes are:

$$H_{COM}(\phi_1) = J_{COM} (\sigma_{\phi_1}^1 \sigma_{\phi_1}^2 + \sigma_{\phi_1}^2 \sigma_{\phi_1}^3 + \sigma_{\phi_1}^1 \sigma_{\phi_1}^3) \quad (\text{S9})$$

$$H_{Br}(\phi_2) = J_{Br} \sigma_{\phi_2}^1 \sigma_{\phi_2}^3 \quad (\text{S10})$$

where

$$J_i = \frac{\Omega_i^2 \eta_i^2 \omega_i}{\Delta_i^2 - \omega_i^2} \quad (\text{S11})$$

determines the coupling strength of the spin-spin interaction due to vibrational mode i . This equation allows for separate pairs of light fields to drive each mode simultaneously, which can therefore have different coupling strengths and detunings. This is required because we wish to be able to precisely control the relative strengths A_i , which can be achieved by changing the relative strengths of the laser fields. Separate pairs of light fields are also necessary since we require the ability to individually set the phase ϕ_i determined by the phase difference between the laser fields in each pair.

S2.3 Ideal experimental behavior of the proposed walks

Now that we have established the Hamiltonians to drive the quantum walks, given by equations (S9) and (S10), we will examine the walk dynamics that we wish to explore. A key observation is that the operators $J \sigma_\phi^m \sigma_\phi^n$ ($m, n \in \{1, 2, 3\}, m \neq n$) leaves invariant the subspace spanned by the following four spin states

$$|1\rangle \equiv |\uparrow, \downarrow, \downarrow\rangle, \quad |2\rangle \equiv |\downarrow, \uparrow, \downarrow\rangle, \quad |3\rangle \equiv |\downarrow, \downarrow, \uparrow\rangle, \quad |4\rangle \equiv |\uparrow, \uparrow, \uparrow\rangle.$$

In order to see this, consider the following decomposition ($m, n \in \{1, 2, 3\}, m \neq n$):

$$\sigma_\phi^m \sigma_\phi^n = (\cos \phi \sigma_x^m + \sin \phi \sigma_y^m) (\cos \phi \sigma_x^n + \sin \phi \sigma_y^n) \quad (\text{S12})$$

in terms of the creation and annihilation operators $\sigma_\pm^m = \sigma_x^m \pm i \sigma_y^m$. It follows that:

$$\sigma_\phi^m \sigma_\phi^n = e^{-2i\phi} \sigma_+^m \sigma_+^n + e^{2i\phi} \sigma_-^m \sigma_-^n + \sigma_+^m \sigma_-^n + \sigma_-^m \sigma_+^n \quad (\text{S13})$$

Here $|n\rangle$ and $|m\rangle$ are coupled by the real strength J , whereas $|4\rangle$ is coupled to the remaining site by the same strength multiplied with the phase $e^{-2i\phi}$. Now, notice that the modes H_{COM} and

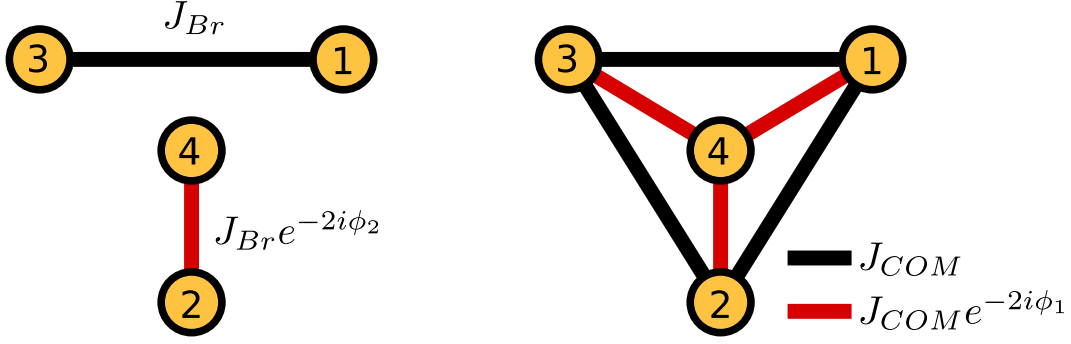


Fig. S4: Networks describing the modes H_{Br} (left) and H_{COM} (right).

H_{Br} are built from operators of the above form. Using these models we can realize quantum walks on the four sites given above. Now one determines the parameters of the quantum walk Hamiltonians:

$$H^{(k)} = \sum_k \sum_{n,m=1}^4 J_{nm}^{(k)} |n\rangle \langle m| \quad \text{with} \quad J_{nm}^{(k)} = \bar{J}_{mn}^{(k)},$$

where the index k refers to the two different modes $H_{COM}(\phi_1)$ and $H_{Br}(\phi_2)$. Figure S4 shows the general situation.

The values to be used for the experiment are given in the following table:

	J_{COM}	J_{Br}	ϕ_1	ϕ_2
H_{CQW_1}	2	-3	$\pi/2$	0.304π
H_{CQW_2}	2	-3	$\pi/2$	-0.304π
H_{QW}	-2	1	$\pi/2$	0

The parameter ϕ_2 is determined by $\cos 2\phi_2 = -1/3$. Since the effect ϕ_1 is just a minus sign in H_{COM} for the edges incident to $|4\rangle$, we see that H_{CQW_1} and H_{CQW_2} are the images of each other under TRS transformation. One can also check that H_{QW} is the time-reversal symmetric counterpart of the chiral walks in that all its couplings are real and equal to the absolute values of the chiral walks after we relabel sites $|2\rangle$ and $|4\rangle$. Computer simulation (Figure S5) shows the effect of TRS breaking, since $P_{1 \rightarrow 2}(t) \neq P_{2 \rightarrow 1}(t)$, enhancement and suppression of transport as the first maxima of H_{CQW_2} and H_{CQW_1} are of considerably larger

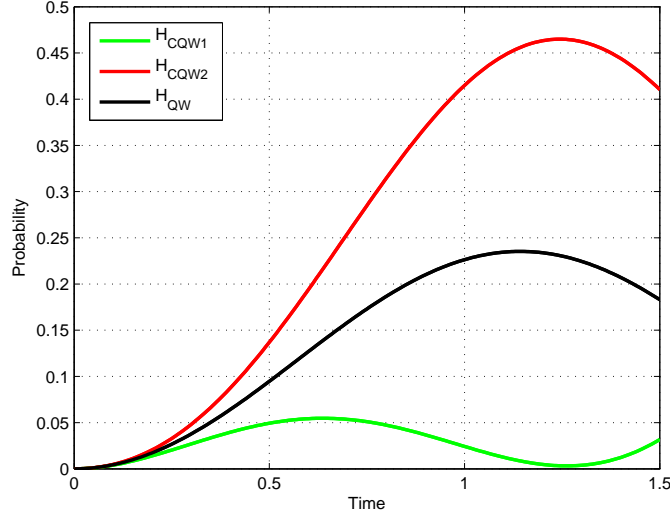


Fig. S5: The effect of the chiral phase parameter on the occupation probability. The plot shows the chiral walkers at site 2 and the achiral one at site 4, all being initially at site 1. By this arrangement the real coupling strengths of the corresponding Hamiltonians are the same.

(smaller) magnitude, respectively, than that of the corresponding symmetric walker. When we compute $P_{2 \rightarrow 1}(t)$, the roles of the two chiral walks are exchanged due to the symmetry of the model.

S2.4 Experimental details

As a specific example we consider using three $^{40}\text{Ca}^+$ ions in a standard linear Paul trap. This atomic species is used by several groups around the world and can be precisely manipulated in the way that we require. Spins can be encoded into a metastable electric quadrupole transition, the excited state of which has a lifetime of approximately 1 second which is much longer than the times required for quantum operations. Spin operations can be driven using a 729nm laser, spin-spin interactions can be implemented using a bichromatic light field with symmetrical detuned sidebands around the electronic transition [24]. We note that implementation of our proposal using another atomic species with a hyperfine transition, for example, would also be

possible.

Figure S6 shows one possibility allowing simultaneous realisation of the Hamiltonians given in equations (S9) and (S10). Two pairs of bichromatic fields are turned on, one pair tuned close to the axial COM and another to the axial breathing mode. We choose to use the axial modes, since they are well-spaced out in frequency, thereby enabling each bichromatic light field to be simultaneously close enough to its nearest vibrational mode such that the effect of that mode completely dominates the spin-spin interaction and sufficiently far away such that the adiabatic approximation still applies.

The criterion to generate a pure spin-spin interaction with each bichromatic field is $|\omega_m - \mu| \gg \eta_m \omega_m$, i.e. the detuning from all sidebands is much greater than the coupling strength on those modes. Using the detunings shown in Figure S6, and $\Omega = 2\pi \times 100 \text{ KHz}$ we obtain ratios $|\omega_m - \mu|/\eta_m \omega_m$ of 21 and 14 for the COM and breathing bichromats, respectively. In this regime, errors due to the generation of phonons are extremely small. Regarding the issue of off-resonant coupling to unwanted modes: straightforward calculations using equation (S11) and the frequencies shown in figure S6 show that in both cases the size of the far-offresonant spin-spin coupling, due to bichromatic field 2 on the COM for example, is more than one order of magnitude less than the desired couplings in every case. This could be further reduced by increasing the frequency separation between axial modes by increasing the confining potential in this direction, for example.

An important experimental consideration is the requirement to maintain a fixed phase relationship between the two pairs of light fields generating the walk Hamiltonians. For example, this can be achieved by generating them in the same acousto-optic modulator (AOM) and thereby keeping their paths common mode, between the point of generation and the point of interaction with the ions. The maximum frequency splitting is approximately 3.4 MHz, which will result in some angular divergence of the different frequencies at the output facet of the

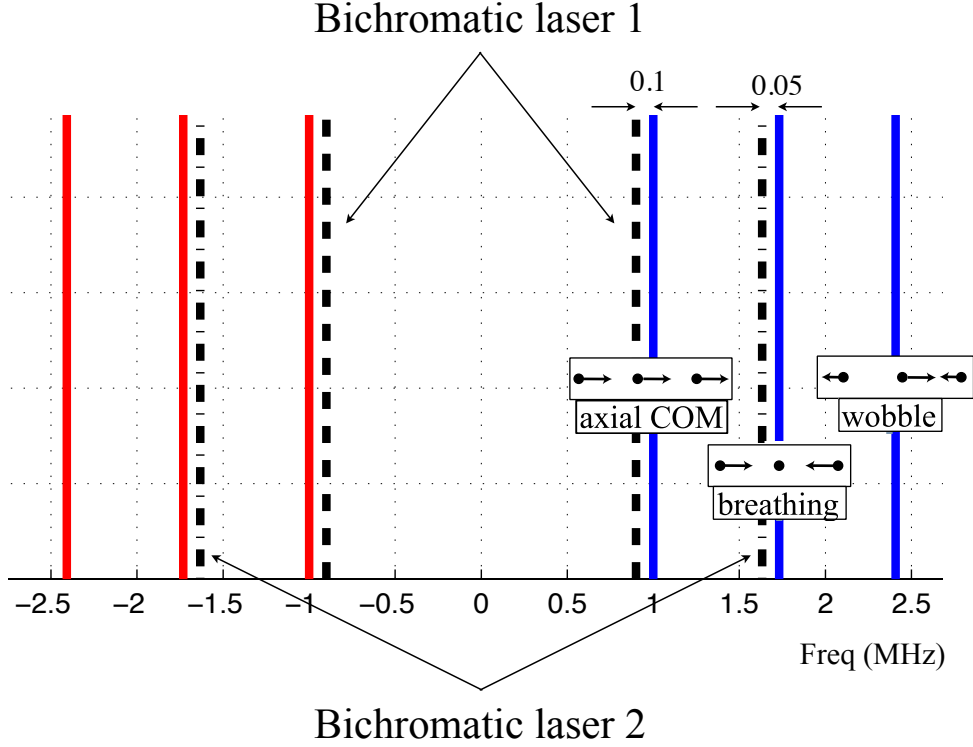


Fig. S6: Mode frequency spectrum of a linear three ion crystal of $^{40}\text{Ca}^+$ in a typical harmonic trap with radial COM (not shown) and axial COM frequencies of 5 MHz and 1MHz, respectively. Two bichromatic laser fields, each symmetrically detuned from the axial COM (by 100KHz) and breathing modes (by 50KHz), drive interactions between spins encoded into an electronic transition of each ion. The phase difference between the spectral components in bichromatic field 1 (2) determines the phase ϕ in the Hamiltonian given in equation (S9) ((S10)).

AOM crystal, which can be compensated with linear optics allowing coupling into an optical fibre for transport to the ion trap itself.

The experiment would proceed as follows. Firstly, standard methods of doppler cooling, resolved sideband cooling on the axial COM and breathing modes, and optical pumping prepares the three ion string into an ultra low entropy state and the initial spin state $|\downarrow, \downarrow, \downarrow\rangle$. Next, a standard combination of single-ion focused and three-ion focused beams is used to prepare the initial state $|\uparrow, \downarrow, \downarrow\rangle$. The bichromatic light fields which implement the desired walk dynamics are then turned on for a fixed period of time. Finally the state of each encoded spin (up

or down) is measured individually using standard fluorescent detection techniques and a CCD camera. Experiments are repeated multiple times from which estimates of the probability for finding spins in all configurations can be deduced.

S3 Fenna-Matthews-Olson complex

The Fenna-Matthews-Olson (FMO) complex is a well studied light harvesting system in green sulfur bacteria. The interest in FMO resides in the high efficiency shown in the transport of energy from the antenna to the reaction center. The faithful description and simulation of the FMO complex has been the highlight of recent research.

The system is composed of three subunits, each made of seven BChl-*a* molecules embedded in a protein scaffold. We restrict our study to the simulation of the exciton transport in a single unit. To simulate the evolution of the system in the one-excitation manifold, we use the following Liouville equation:

$$\dot{\rho} = \mathcal{L}[\rho] = -i[H, \rho] + \phi \hat{L}_\phi\{\rho\} + \gamma \hat{L}_\gamma\{\rho\} + \tau \hat{L}_\tau\{\rho\} \quad (\text{S14})$$

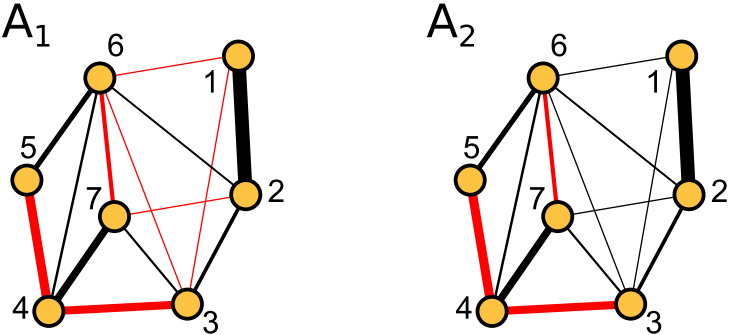
where the Lindblad super-operators are defined as:

$$\hat{L}_\phi\{\rho\} \equiv \sum_n L_{\phi,n} \rho L_{\phi,n}^\dagger - \frac{1}{2} \left(L_{\phi,n}^\dagger L_{\phi,n} \rho + \rho L_{\phi,n}^\dagger L_{\phi,n} \right) \quad L_{\phi,n} = |n\rangle\langle n| \quad (\text{S15})$$

$$\hat{L}_\gamma\{\rho\} \equiv \sum_n L_{\gamma,n} \rho L_{\gamma,n}^\dagger - \frac{1}{2} \left(L_{\gamma,n}^\dagger L_{\gamma,n} \rho + \rho L_{\gamma,n}^\dagger L_{\gamma,n} \right) \quad L_{\gamma,n} = |d\rangle\langle n| \quad (\text{S16})$$

$$\hat{L}_\tau\{\rho\} \equiv \sum_{n \in T} L_{\tau,n} \rho L_{\tau,n}^\dagger - \frac{1}{2} \left(L_{\tau,n}^\dagger L_{\tau,n} \rho + \rho L_{\tau,n}^\dagger L_{\tau,n} \right) \quad L_{\tau,n} = |\tau\rangle\langle n| \quad (\text{S17})$$

where the sums are over the site basis and T is the set of sites connected to the reaction center (in this case only site three). The coherent part of the evolution is described using a time reversal symmetric Hamiltonian from the literature [25]. In (S14) the non-coherent terms describe the coupling of the system with a thermal bath, dephasing, Eq. (S15), and recombination, Eq. (S16),



Edges	A_1	variance	A_2	variance
3-4	1.31484899π	$4.33 \cdot 10^6 \pi$	1.58371001π	$4.86 \cdot 10^6 \pi$
4-5	1.66997830π	$5.20 \cdot 10^6 \pi$	1.39551582π	$6.60 \cdot 10^6 \pi$
6-7	1.8406103π	$1.25 \cdot 10^5 \pi$	0.1338368π	$1.72 \cdot 10^5 \pi$
2-7	1.2949616π	$2.80 \cdot 10^5 \pi$		
1-6	1.67543320π	$5.36 \cdot 10^6 \pi$		
1-3	0.04222214π	$4.36 \cdot 10^6 \pi$		
3-6	0.8761298π	$1.03 \cdot 10^5 \pi$		

Table S1: Transport enhancement in the FMO complex. Both for A_1 and A_2 , complex phases are applied to the red edges. The results of a simultaneous optimization procedure are listed in the table.

and the effect of the excitation trapping at the site connected to the reaction center, Eq. (S17). The thermal bath, for the present paper, is considered as a set of harmonic oscillators coupled to the system of interest as in [15, 11].

The initial state is set on site one and the reaction center is connected as an energy sink to site three. In the simulation we use a dephasing rate of $\phi = 9.0 \text{ ps}^{-1}$ (which corresponds to 295K), the recombination rate is $\gamma = 1 \text{ ns}^{-1}$ and trapping rate from site three to the reaction center is $\tau = 1.0 \text{ ps}^{-1}$.

The optimization of the phases was found to be robust with respect to phase changes. The resulting phases are reported in Table S1.

S4 Small-world networks

The Watts-Strogatz model [17] gives a constructive algorithm for building a network with small-world characteristics, starting from a regular lattice. The latter is defined as a periodic chain of N nodes where each node is connected to k neighbors ($k/2$ to the left and $k/2$ to the right). The final small-world network is obtained by taking all neighboring edges at each node and rewiring all the edges toward the node left with a probability p . The limit for $p \rightarrow 1$ of the Watts-Strogatz model is the Erdős-Rényi random model with fixed number of edges (restricted to connected graphs).

In our case, we set $N = 32$ and $k = 4$ and choose only connected graphs as we are concerned in comparing transport on networks of the same sites. The initial state is on site S while the sink is a external site connected to site E . Site E latter is placed on the opposite side of the initial circle. The absorption rate of the sink is $r = 1.0$. The evolution is described by the coherent Hamiltonian, which, in this case, corresponds to the connectivity matrix of the network. We define $\tau_{1/2}^{QW}$ the time needed by the normal quantum walker to reach the probability $p_{sink}(t) = 1/2$. We add phases to the edges neighboring node E and optimize them in order to improve the probability of being trapped in the target site at time $\tau_{1/2}^{QW}$. The non-coherent part (trapping) is described by a Lindbladian super-operator. We repeat the evolution for 200 different realizations of the graph for each value of p .

S5 Numerical Methods

We used the Quantum Information Toolkit, primarily developed by Ville Bergholm. This is a toolkit for the Matlab programming language. The optimization procedure used in the FMO and the Watts-Strogatz examples rely on the *Interior-point Optimization* algorithm of the Matlab minimization toolkit. We start the optimization procedure several times from different randomly

chosen points of the parameter space, to reach the global minimum of cost function with more certainty. Source code for all simulations done in this work is available upon request.